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Synthesis and Structural Study of Metal-Organic Complexes Formed by Rare-Earths and Triazole Ligand

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Metal-organic complex systems have demonstrated high efficiency in various areas of technology, such as catalysis and exploration of their magnetic properties[1]. Knowing these complexes consist of metal centers linked to organic ligands, the focus of this work is the synthesis and characterization of compounds formed by the combination of 1-(4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylic acid (ACNO2) and rare-earth metals ions. The synthesis of these complexes was achieved by subjecting an One-pot mixture of 0.05 mmol of ACNO2 and 0.05 mmol of $Ln(NO_3)_3 \cdot xH_2O$ (Ln=La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb) in an ethanolic solution to an ultrasonic bath for 10 minutes. After that, the mixtures were allowed to rest for some days, forming needle crystals. The crystals were measured using Bruker D8 Venture diffractometer with KαMo radiation (λ = 0.71073 Å), and refined using the SHELX-2019 program package. The refinement of the structures yielded statistical data with wR=0.0523, S=1.100, R=0.0212 for the La compound; wR=0.0784, S=1.058, R=0.0387 for the Ce compound; wR=0.0940, S=1.032, R=0.0427 for the Pr compound; wR=0.0825, S=1.046, R=0.0380 for the Nd compound; wR=0.0641, S=1.048, R=0.0367 for the Sm compound; wR=0.0503, S=1.094, R=0.0231 for the Eu compound; wR=0.0449, S=1.122, R=0.0196 for the Gd compound; wR=0.0475, S=1.092, R=0.0198 for the Tb compound; wR=0.0571, S=1.078, R=0.0256 for the Dy compound; wR=0.0478, S=1.070, R=0.0204 for the Ho compound; wR=0.0717, S=1.079, R=0.0353 for the Er compound. From the statistical parameters and structural analysis, it was observed that the complexes belong to the trigonal crystalline system with the space group number 147, $P\bar{3}$. The Tm and Yb compounds were further characterized by powder analysis. The obtained compounds may exhibit certain aspects and utilities that will be tested further: concerning luminescence, as suggested in literature for similar ones[1], and in terms of single-ion magnetism properties.

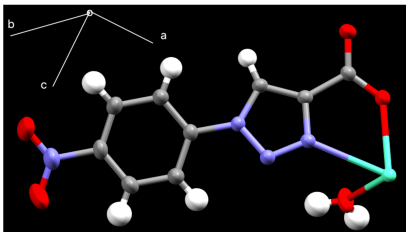

Figure 1: Complexes Asymmetric Unit

Acknowledgments: Agir UFF, CNPq, Proppi UFF, Faperj

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